Mathematisches Forschungsinstitut Oberwolfach

Report No. 19/2021

DOI: 10.4171/OWR/2021/19

Small Collaboration: Modeling Phenomena from Nature by Hyperbolic Partial Differential Equations (hybrid meeting)

Organized by
Christian Klingenberg, Würzburg
Qin Li, Madison
Marlies Pirner, Würzburg

11 April – 17 April 2021

Abstract. Nonlinear hyperbolic partial differential equations constitute a plethora of models from physics, biology, engineering, etc. In this workshop we cover the range from modeling, mathematical questions of well-posedness, numerical discretization and numerical simulations to compare with the phenomenon from nature that was modeled in the first place. Both kinetic and fluid models were discussed.

Mathematics Subject Classification (2010): 35B40, 35L65, 35Q20, 35R30, 65M06, 76W05, 82C40.

Introduction by the Organizers

The workshop (held in a hybrid format) titled *Modeling Phenomena from Nature by Hyperbolic Partial Differential Equations*, organized by Christian Klingenberg (Würzburg, Germany), Qin Li (Madison, Wisc., USA) and Marlies Pirner (Würzburg, Germany) was attended by 18 participants, 9 of which were female.

Nonlinear hyperbolic systems of time-dependent partial differential equations are important mathematical models for a large number of complex natural systems of fundamental interest. The governing equations can be derived from first principles. In applications these models are used with great success.

In this workshop we spanned the gamut from modeling physical phenomena by hyperbolic partial differential equations, discussing questions of existence, uniqueness and well-posedness, their numerical discretization and related numerical analysis and numerical implementation questions to numerical simulations in order to ascertain how this matches the physical phenomenon at hand.

Depending on the time scale and spatial scale in the application at hand, the models may be either microscopic kinetic equations or a macroscopic fluid equations. Both types of models were discussed. Next we list some of those topics.

Kinetic models

Here we take an atomistic view of the flow. Considering density distributuons of these micrsoscopically interacting particles, we obtain Boltzmann-type equations consisting of a first order transport operator for the density distribution of the particles which are set equal to a zeroth order term describing the interaction between the particles. As reported on by Marlies Pirner, she *models gas mixtures* in this way, see e.g. [1], and proves that this model satisfies physical properties. The numerical implementation of this new model needs to be found. Seok-Bae Yun and Gi-Chan Bae reported on theoretical aspects of certain kinetic models, which lend itself to efficient numerical simulations, while still modeling the physics appropriately.

For a kinetic model of plasma, the Vlasov-Poisson model, enhanced by a BGK relaxation term, aspects of Landau damping were discussed by Lena Baumann.

The study of *uncertainty quantification* for kinetic models was discussed, see here [2]. But uncertainty quantification does not always represent the viewpoint of the experimentalists. Instead they want to determine the uncertain coefficient in a PDE by measuring the solution at the parts of the boundary, given data on other parts of the boundary. The lectures of Ru-Yu Lai introduced and reported new results on this subject. In other words experimentalists are interested in solving the *inverse problem* in a Bayesian setting, see here [3] for a related question. We followed on from this by considering a model from mathematical biology, namely the motion of cells, as described by the kinetic chemotaxis equations. The corresponding macroscopic Keller-Segel type model will be a diffusion equation. This was reported on by Min Tang. The aim is to study the inverse problems for these two settings. Kathrin Hellmuth reported on these ideas, see [11].

Numerical methods for kinetic equations that continue to be valid in the limit of Knudsen number going to zero are called asymptotic preserving. In addition we found numerical methods that at the same preserve stationary solutions, see here [4], as repoted on by Farah Kanbar. It was discussed on how to extend this to kinetic models of gas mixtures.

Finally kinetic models for multi-species *quantum particles* are devised and existence is proven see here [5]. It was discussed how this can be translated to numerical schemes. This was reported on by Sandra Warnecke.

The Euler equations of compressible gas dynamics, theory

In one space dimension one has an understanding of existence and uniqueness of solutions to the compressible Euler equations. In that situation (under appropriate assumptions) a sequence of approximations to the Euler equations converges to the weak solutions of Euler equations. In higher space dimensions much less is understood, see here [6] and here [7]. Simon Markfelder reported on this circle of

ideas. Most likely weak solutions are not the appropriate solution concept here. The goal is to identify a proper notion for solutions. Eduard Feireisl studied this in two lectures in the context of stochastics. Solution concepts of the compressible multi-dimensional Euler equations may also be studied by looking at limits of numerical approximations. This was reported on by Eva Horlebein.

The Euler equations of compressible gas dynamics, numerics

Numerics of conservation laws has been dominated by the idea of Godunov, where a crucial ingredient has been the propagation of discontinuous data, the Riemann problem. This is a one-space-dimensional idea. It seems it is time for a change of paradigm. Following a suggestion of Phil Roe, in multiple space dimensions the evolution of continuous finite elements by using (almost) exact evolution at discrete points seems to be very promising, see here [8]. The study of such *genuinely multi-dimensional schemes* holds enormous promise, because they naturally satisfy all involution constraints. Progress towards this was presented by Wasilij Barsukov.

For the *Euler equations with gravity* we seek numerical methods that are both asymptotic preserving in the low Mach limit and also stationary preserving, also know as well-balanced, see here [9], or here [10]. Ways on how to improve numerical schemes that combine these two features were reported on by Claudius Birke and Philipp Edelmann.

Overall this workshop gave space to discuss the above circle of ideas in the wonderful atmosphere of Oberwolfach.

References

[1] J. Haack, C. Hauck, C. Klingenberg, M. Pirner, S. Warnecke, *A consistent BGK model with velocity-dependent collision frequency for gas mixtures*, submitted 2021, see paper here

[2] Herzing, T., Klingenberg, C., Pirner, M.: *Hypocoercivity of the linearized BGK-equation with stochastic coefficients*, submitted (2020), see paper here

[3] Klingenberg, C., Lai, R., Li, Q.: *Reconstruction of the emission coefficient in the nonlinear radiative transfer equation*, SIAM Journal on Applied Mathematics, Vol. 81, 1 (2021) see the paper here

[4] Emako, F. Kanbar, C. Klingenberg, M. Tang, *A criterion for asymptotic preserving schemes of kinetic equations to be uniformly stationary preserving*, submitted (2021) see paper here

[5] G. Bae, C. Klingenberg, M. Pirner. S. Yun: *BGK model of the multi-species Uehling Uhlenbeck equation*, Kinetic and Related Models, Vol. 14, Issue 1 (2021) see paper here

[6] Feireisl, E., Klingenberg, C., Kreml, O., Markfelder, S.: *On oscillatory solutions to the complete Euler equations*, Journal of Differential Equations, Vol. 296, issue 2, pp 1521-1543, (2020), see paper here

[7] E. Feireisl; C. Klingenberg; S. Markfelder, 'On the density of wild initial data for the compressible Euler system', Calculus of Variations (2020), see paper here

[8] Wasilij Barsukow; Jonathan Hohm; Christian Klingenberg; Philip L Roe, *The active flux scheme on Cartesian grids and its low Mach number limit*, Journal of Scientific Computing, vol. 81, pp. 594-622, (2019), see paper here

[9] Berberich, J., Käppeli, R., Chandrashekar, P., Klingenberg, C.: *High order discretely well-balanced methods for arbitrary hydrostatic atmospheres*, Communications in Computational Physics (2021), see paper here

[10] Edelmann, Horst, Berberich, Andrassy, Higl, Klingenberg, Röpke: *Well-balanced treatment of gravity in astrophysical fluid dynamics simulations at low Mach numbers*, submitted 2021 see paper here

[11] Helmuth, K., Klingenberg, C., Li, Q., Tang, M.: *Multiscale convergence of the inverse problem for chemotaxis in the Bayesian setting*, in the volume *Inverse Problems with Partial Data* edited by Qin Li and Li Wang, submitted to *Computation* (2021)

Acknowledgement: We thank the MFO for generously supporting this workshop by awarding OWLG grants in addition to VCA grants to on-site participants of this workshop.

Small Collaboration (hybrid meeting): Modeling Phenomena from Nature by Hyperbolic Partial Differential Equations

Table of Contents

Seok-Bae Yun (joint with Doheon Kim, Myeong-Su Lee)
Entropy production estimate for the ES-BGK model with the correct Prandtl number 1053

Marlies Pirner (joint with Jeff Haack, Cory Hauck, Christian Klingenberg, Sandra Warnecke)
On multi-species BGK models with velocity dependent collision frequencies 1054

Farah Kanbar (joint with Christian Klingenberg, Min Tang)
A criterion for asymptotic preserving schemes of kinetic equations to be uniformly stationary preserving 1057

Claudius Birke (joint with Christophe Chalons, Christian Klingenberg)
A low Mach well-balanced relaxation scheme for the compressible Euler equations with gravity 1058

Min Tang
Individual based models for bacterial movement exhibiting Lévy-flight type movement induced by intra-cellular noise 1060

Lena Baumann (joint with Christian Klingenberg, Marlies Pirner)
On Landau damping coupled with relaxation for the Vlasov-Poisson-BGK equation for small collision frequencies 1060

Philipp V. F. Edelmann (joint with Leonhard Horst, Jonas P. Berberich, Robert Andrassy, Johann Higl, Giovanni Leidi, Christian Klingenberg, Friedrich K. Röpke)
Well-balanced treatment of gravity in astrophysical fluid dynamics simulations at low Mach numbers 1062

Wasilij Barsukow
Approximate evolution operators for the Active Flux method 1063

Eduard Feireisl (joint with F. Fanelli)
Statistical solutions to the barotropic Navier-Stokes system 1067

Simon Markfelder
Convex integration applied to the compressible Euler equations 1068

Eva Horlebein (joint with Eduard Feireisl, Christian Klingenberg, Simon Markfelder)
On convergence of the invariant domain preserving scheme by Jean-Luc Guermond and Bojan Popov to a dissipative measure-valued solution in the case of the complete Euler equations 1069

Ru-Yu Lai (joint with Qin Li, Gunther Uhlmann, and Yang Yang)
Introduction to Inverse Problems and Transport Equations I and II 1071

Gi-Chan Bae (joint with Seok-Bae Yun)
Shakhov model near a global Maxwellian 1074

Sandra Warnecke (joint with Christian Klingenberg, Marlies Pirner)
Numerical schemes for multi-species (quantum) BGK equations 1077

Eduard Feireisl (joint with F. Fanelli, M. Hofmanova)
Ergodic theory for energetically open compressible fluid flows 1079

Qin Li (joint with Ke Chen, Shi Chen, Christian Klingenberg, Ru-Yu Lai, Jianfeng Lu, Gunther Uhlmann, Stephen Wright)
Low rank structure in the forward and inverse kinetic theory 1079

Kathrin Hellmuth (joint with Christian Klingenberg, Qin Li, Min Tang)
An inverse problem for chemotaxis 1080

Abstracts

Entropy production estimate for the ES-BGK model with the correct Prandtl number

Seok-Bae Yun
(joint work with Doheon Kim, Myeong-Su Lee)

In this talk, we establish the entropy-entropy production estimate for the ES-BGK model, a generalized version of the BGK model of the Boltzmann equation introduced for better approximation in the Navier-Stokes limit:

$$\partial_t f + v \cdot \nabla_x f = A_\nu(\mathcal{M}_\nu(f) - f). \tag{1}$$

The non-negative function $f(x, v, t)$ is the velocity distribution function on $(x, v) \in \Omega \times \mathbb{R}^3$ in the phase space at time $t \geq 0$ ($\Omega \in \mathbb{R}^n$). A_ν is the collision frequency.

The ellipsoidal Gaussian (or non-isotropic Gaussian) is defined by

$$\mathcal{M}_\nu(f) := \frac{\rho}{\sqrt{\det(2\pi\mathcal{T}_\nu)}} \exp\left(-\frac{1}{2}(v-U)^\top \mathcal{T}_\nu^{-1}(v-U)\right),$$

where ρ, U, and T denote the the local density ρ, the local bulk velocity U and the local temperature T respectively, and the temperature tensor $\mathcal{T}_\nu$ is given by

$$\mathcal{T}_\nu = (1-\nu)TI + \nu\Theta. \qquad (-1/2 \leq \nu < 1)$$

Here, I denotes the 3-by-3 identity matrix, and Θ is the stress tensor:

$$\Theta(t,x) = \frac{1}{\rho}\int_{\mathbb{R}^3} f(x,v,t)(v-U)\otimes(v-U)dv.$$

To state the main result, we define the H-functional $H(f)$, the relative entropy $H(f|g)$, and the entropy production functional $D_\nu(f)$ as follows:

$$\begin{aligned} H(f) &= \int_{\mathbb{R}^3} f\ln f dv, \qquad H(f|g) = \int_{\mathbb{R}^3} f\ln(f/g)dv, \\ D_\nu(f) &= \int_{\mathbb{R}^3} A_\nu(\mathcal{M}_\nu - f)\ln f dv. \end{aligned} \tag{2}$$

Then our main result is as follows:

Theorem. Let $-1/2 \leq \nu < 1$. Assume that the solution f to (1) is regular enough so that the functionals in (2) are well-defined, and satisfies $\rho(x,t) > 0$ for a.e. x, t. Define C_ν for $-1/2 \leq \nu < 1$ by

$$C_\nu = \sup_{x>0} \frac{3\ln\left(1+\frac{1}{3}x\right) - \ln\left(1+\frac{1+2\nu}{3}x\right) - 2\ln\left(1+\frac{1-\nu}{3}x\right)}{3\ln\left(1+\frac{1}{3}x\right) - \ln(1+x)}.$$

Then, we have

(1) C_ν satisfies the following bound:

$$C_\nu \leq \frac{1}{3}\,\nu^2(5-2\nu)$$

on $-1/2 \leq \nu < 1$.

(2) For such choice of C_ν, Cercignani-type entropy-entropy production estimate holds:

$$D_\nu(f) \leq -(1-C_\nu)A_\nu H(f|\mathcal{M}_0)$$

on $-1/2 \leq \nu < 1$.

Our result improves the previous entropy production estimate by Yun [Kinet. Relat. Models **9** (2016), no. 3, 605–619.] in that (1) the full range of Prandtl parameters $-1/2 \leq \nu < 1$ including the critical case $\nu = -1/2$ is covered, and (2) a sharper entropy production bound is obtained. An explicit characterization of the coefficient of the entropy-entropy production estimate is also presented.

On multi-species BGK models with velocity dependent collision frequencies

Marlies Pirner

(joint work with Jeff Haack, Cory Hauck, Christian Klingenberg, Sandra Warnecke)

We consider a BGK-type model for gas mixtures that, in the case of two species, takes the form

$$\begin{aligned} \partial_t f_1 + v\cdot\nabla_x f_1 &= \nu_{11}(M_{11}-f_1)+\nu_{12}(M_{12}-f_1),\\ \partial_t f_2 + v\cdot\nabla_x f_2 &= \nu_{22}(M_{22}-f_2)+\nu_{21}(M_{21}-f_2), \end{aligned} \tag{1}$$

along with appropriate boundary and initial conditions. Here $f_1 = f_1(x,v,t)$ and $f_2 = f_2(x,v,t)$ are the number densities of species of mass m_1 and m_2, respectively, with respect to the phase space measure $dxdv$; $x \in \mathbb{R}^3$ is the position coordinate of phase space; $v \in \mathbb{R}^3$ is the velocity coordinate; and $t \geq 0$ is time. The relaxation operator on the right hand side of (1) involves target functions of the form

$$M_{kj} = \exp(m_k\lambda_0^{kj} + m_k\lambda_1^{kj}\cdot v + m_k\lambda_2^{kj}|v|^2), \tag{2}$$

which depend on parameters $\lambda^{kj} = (\lambda_0^{kj}, \lambda_1^{kj}, \lambda_2^{kj}) \in \mathbb{R}\times\mathbb{R}^3\times(-\infty,0)$, and (non-negative) collision frequencies ν_{kj}. These parameters depend implicitly on f_1 and f_2, and once specified, determine the BGK operator.

In [1], we derive a model of the form (1) that allows for velocity-dependent collision frequencies. Our derivation includes as a by-product the single-species BGK model with velocity-dependent collision frequency that was proposed in [2]. We identify target functions that are consistent with the conservation laws for (1) and satisfy an entropy minimization principle. In particular, *intra-species* collisions

(between the same species) should preserve mass, momentum, and energy within a species; that is,

$$\int m_k \nu_{kk} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} (M_{kk} - f_k) dv = 0, \quad k \in \{1, 2\}. \tag{3}$$

Meanwhile *inter-species* collisions (between different species) should preserve the mass of each species, but only the combined momentum and energy of both; that is,

$$\begin{gathered} \int m_1 \nu_{12} (M_{12} - f_1) dv = 0, \quad \int m_2 \nu_{21} (M_{21} - f_2) dv = 0 \\ \int m_1 \nu_{12} \begin{pmatrix} v \\ |v|^2 \end{pmatrix} (M_{12} - f_1) dv + \int m_2 \nu_{21} \begin{pmatrix} v \\ |v|^2 \end{pmatrix} (M_{21} - f_2) dv = 0. \end{gathered} \tag{4}$$

When the collision frequencies are independent of v, the integrals in (3) and (4) can be computed explicitly, thereby providing relationships between the parameters λ^{kj} and the moments of f_1 and f_2 with respect to $\{1, v, |v|^2\}$. In the single-species case, this relationship defines the target function as the Maxwellian associated to f, while in the multi-species case, additional constraints must be imposed. However, when the collision frequencies depend on v, the aforementioned integrals are not always computable in closed form and the relationship between the parameters λ^{kj} and the moments of f_1 and f_2 with respect to $\{1, v, |v|^2\}$ cannot be written down analytically.

The form of the target functions in (2) can be motivated as solutions to the weighted entropy minimization problem

$$\min_{g \in \chi_i} \int \nu_{ii}(v)(g(v) \ln g(v) - g(v)) dv, \quad i \in \{1, 2\}, \tag{5}$$

where

$$\chi_i = \left\{ g \;\middle|\; g \geq 0,\, \nu_{ii}(v)(1 + |v|^2) g \in L^1(\mathbb{R}^3),\, \int m_k \nu_{ii}(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} (g(v) - f_i(v)) dv = 0 \right\}.$$

The choice of the set χ_i ensures the conservation of mass, momentum and energy for intra-species collisions. Correspondingly, the form of the mixed target functions (2) can be seen as a solution to the weighted entropy minimization problem

$$\min_{g_1, g_2 \in \chi_{12}} \int \nu_{12}(g_1 \ln g_1 - g_1) dv + \int \nu_{21}(g_2 \ln g_2 - g_2) dv, \tag{6}$$

where

$$\chi_{12} = \Bigg\{ (g_1, g_2) \;\Big|\; g_1, g_2 > 0,\, \nu_{12}(1+|v|^2)g_1,\, \nu_{21}(1+|v|^2)g_2 \in L^1(\mathbb{R}^3),$$
$$\int m_1\nu_{12}g_1 dv = \int m_1\nu_{12}f_1 dv, \quad \int m_2\nu_{21}g_2 dv = \int m_2\nu_{21}f_2 dv,$$
$$\int m_1\nu_{12}\begin{pmatrix} v \\ |v|^2 \end{pmatrix}(g_1 - f_1)dv + \int m_2\nu_{21}\begin{pmatrix} v \\ |v|^2 \end{pmatrix}(g_2 - f_2)dv = 0 \Bigg\}.$$

The set χ_{12} ensures the conservation of mass for each species, total momentum and total energy for inter-species collisions. The consistency of the presented model and an H-Theorem are given in the following theorems. The proof of both theorems can be found in [1].

Theorem 1. *There exist unique λ_1, λ_2, λ_{12} and λ_{21} such that mass, total momentum and total energy are conserved, which means*

$$\int \nu_{ii}(M_{ii} - f_i)\, m_1 \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = 0 \quad \textit{for} \quad i = 1, 2 \tag{7}$$

and

$$\begin{gathered} \int \nu_{12}(M_{12} - f_1)dv = 0, \qquad \int \nu_{21}(M_{21} - f_2)dv = 0 \\ \int \nu_{12}\begin{pmatrix} m_1 v \\ \frac{m_1}{2}|v|^2 \end{pmatrix}(M_{12} - f_1)dv = -\int \nu_{21}\begin{pmatrix} m_2 v \\ \frac{m_2}{2}|v|^2 \end{pmatrix}(M_{21} - f_2)dv. \end{gathered} \tag{8}$$

Theorem 2. *Assume $f_1, f_2 > 0$ and that (7) and (8) hold. We define the function $h(z) = z\ln(z) - z$ and the total entropy $H(f_1, f_2) = \int (h(f_1) + h(f_2))dv$. Then the following entropy inequality holds true:*

$$\partial_t H(f_1, f_2) + \nabla_x \cdot \left[\int v(h(f_1) + h(f_2))dv \right] \leq 0,$$

with equality if and only if f_1 and f_2 are two Maxwellian distributions with the same mean velocities and temperatures.

References

[1] Haack, J., Hauck, C., Klingenberg, C., Pirner, M., Warnecke, S. (2021). A consistent BGK model with velocity-dependent collision frequency for gas mixtures. arXiv preprint arXiv:2101.09047.

[2] Struchtrup, H. (1997) . The BGK-model with velocity-dependent collision frequency. Continuum Mechanics and Thermodynamics, 9. Jg., Nr. 1, S. 23-31.

A criterion for asymptotic preserving schemes of kinetic equations to be uniformly stationary preserving

Farah Kanbar

(joint work with Christian Klingenberg, Min Tang)

In this work we are interested in the stationary preserving property of asymptotic preserving (AP) schemes for kinetic models. We introduce a criterion for AP schemes for kinetic equations to be uniformly stationary preserving (SP). Our key observation is that as long as the Maxwellian of the distribution function can be updated explicitly, such AP schemes are also SP. To illustrate our observation, three different AP schemes for three different kinetic models are considered. Their SP property is proved analytically and tested numerically, which confirms our observations.

Kinetic Model	Scheme	Reference
Neutron transport equation	Parity-equations based	[1]
Chemotaxis kinetic model	UGKS	[2, 3, 4]
Boltzmann equation	IMEX Penalization method	[5]

Table 1. A list of kinetic models together with their corresponding schemes.

Example of a kinetic model

The neutron transport equation,

$$\partial_t f + \frac{1}{\varepsilon} v \cdot \nabla_x f = \frac{1}{\varepsilon^2}(\frac{1}{2}\int_{-1}^{1} f dv' - f) \tag{1}$$

As $\varepsilon \to 0$, $f(x, v, t) \to \rho_0(x, t)$ which solves the diffusion equation,

$$\partial_t \rho_0 - \partial_x(\frac{1}{3\sigma_T}\partial_x \rho_0) + \sigma_a \rho_0 = q. \tag{2}$$

AP schemes

A scheme is AP, if when the Knudsen number (ε) goes to zero in the discretized scheme, it converges to a good discretization of the corresponding limit model.

SP schemes

We call a scheme is SP if the following two requirements are satisfied:

- The discrete stationary solution provides a good approximation for the steady state solution.
- Starting from a discrete stationary solution, the solution of the time evolutionary problem does not change.

The criterion

As long as the Maxwellian of the distribution function can be updated explicitly and the discretization linearly depends on the Maxwellian, such Asymptotic Preserving (AP) schemes are also Stationary Preserving (SP).

References

[1] S. Jin, *Asymptotic preserving (AP) schemes for multiscale kinetic and hyperbolic equations: a review*, Riv. Mat. Univ. Prama **3** (2012), 177–216.

[2] L. Mieussens, *On the asymptotic preserving property of the unified gas kinetic scheme for the diffusion limit of linear kinetic models*, Journal of Computational Physics **253** (2013), 138–156.

[3] Kun Xu, *A Gas-Kinetic BGK Scheme for the Navier-Stokes Equations and Its Connection with Artificial Dissipation and Godunov Method* , Journal of Computational Physics **171(1)** (2001), 289–335.

[4] Kun Xu and Juan-Chen Huang, *A unified gas-kinetic scheme for continuum and rarefied flows*, Journal of Computational Physics **229(20)** (2010), 7747–7764.

[5] F. Filbet and S. Jin, *A class of asymptotic-preserving schemes for kinetic equations and related problems with stiff sources*, Journal of Computational Physics **229(20)** (2010), 7625–7648.

A low Mach well-balanced relaxation scheme for the compressible Euler equations with gravity

Claudius Birke

(joint work with Christophe Chalons, Christian Klingenberg)

1. The Euler equations

The flow of an compressible inviscid fluid can be described by the Euler equations. For one space dimension these equations are defined in non-dimensional form by

$$\begin{aligned} \partial_t \rho + \partial_x \rho u &= 0, \\ \partial_t \rho u + \partial_x (\rho u^2 + \frac{1}{M^2} p) &= -\frac{1}{M^2} \rho \partial_x \phi, \\ \partial_t E + \partial_x (E + p) u &= -\rho u \partial_x \phi. \end{aligned} \tag{1}$$

In this dimensionless formulation, M represents the Mach number, which controls the ratio between the velocity of the gas and the speed of sound. Depending on the application, the flows can have large scale differences, e.g. the sound speed can be much higher than the speed of the fluid flow. In these low Mach number regimes standard finite volume schemes suffer from excessive diffusion, which can erase the structure of the solution beyond recognition.

When studying the Euler equations with gravity source terms, one also has to consider their influence on the behaviour of steady states. In several applications like astrophysics one deals with problems close to the hydrostatic equilibrium

$$\begin{cases} u = 0, \\ \partial_x p = -\rho \partial_x \phi. \end{cases} \tag{2}$$

Numerical schemes do not automatically satisfy a discrete equivalent of (2). As a result these steady states are not preserved exactly by such schemes and small perturbations around the equilibrium cannot be resolved unless the resolution of the scheme is increased.

Therefore special care must be taken when constructing numerical methods for problems with low Mach numbers or close to hydrostatic equilibrium.

2. The Relaxation Model

The main idea of the relaxation approach is to approximate the solution of the original system, here (1), by the solution of an extended relaxation system that includes relaxation source terms. In the limit of the relaxation parameter, this relaxation system is consistent with the original system. The relaxation models are hyperbolic with only linearly degenerated characteristic fields, so that the associated Riemann problem is easy to solve and efficient Godunov-type methods based on approximate Riemann solvers can be constructed.

Inspired by the two-speed relaxation model introduced by Chalons *et al.* in [1] for the barotropic, homogeneous Euler equations, we approximate the Euler equations (1) by the new relaxation model

$$
\begin{aligned}
\partial_t \rho + \partial_x (\rho v) &= 0,\\
\partial_t (\rho u) + \partial_x \left(\rho u v + \frac{\pi}{M^2}\right) &= -\rho \partial_x Z,\\
\partial_t E + \partial_x ((E+\pi) v) &= -\rho v \partial_x Z,\\
\partial_t (\rho \pi) + \partial_x (\rho \pi v) + ab \partial_x v &= \rho \frac{p-\pi}{\varepsilon},\\
\partial_t (\rho v) + \partial_x \left(\rho v^2\right) + \frac{a}{b} \partial_x \frac{\pi}{M^2} &= \rho \frac{u-v}{\varepsilon} - \frac{a}{b} \rho \partial_x Z,\\
\partial_t \rho Z + \partial_x \rho v Z &= \rho \frac{\phi - Z}{\varepsilon},
\end{aligned}
\tag{3}
$$

where the relaxation variables π, v and Z relax the pressure p, the velocity u and the gravitational potential ϕ. The solutions of this model can be seen as a viscous approximation of the solutions of the original system (1) as long as the subcharacteristic conditions

$$
a \geq b \quad \text{and} \quad ab \geq \rho^2 c^2 \tag{4}
$$

are satisfied. While in a classical Suliciu-type relaxation model only one relaxation speed is used, here it is divided into two speeds $a > 0$ and $b > 0$. This is useful to control viscosity for density and velocity separately. Choosing the scalings $a \sim \mathcal{O}(M^2)$ and $b \sim \mathcal{O}(1)$ for the speeds, the viscosity on the velocity u remains bounded, which is the key to obtain accurate solutions in the low Mach limit. By adding the transport relaxation equation for the gravitational potential, the Riemann problem associated to the relaxation system becomes under-determined. This failure can be used to introduce an additional closure equation, that is a discretization of the steady state condition in (2). By using this closure equation to determine the approximate Riemann solver, the solver is automatically able

to preserve steady states at rest [2]. The resulting approximate Riemann solver additionally ensures the positivity of the density and satisfies a discrete entropy inequality. Building on this inequality, it can be proven that for steady and space periodic solutions, the solutions for velocity and pressure are constant in space, so that no unphysical checkerboard modes can occur. On the basis of the approximate Riemann solver, a Godunov-type finite volume method for solving the original Euler equations can be constructed. This method inherits the properties of the approximate Riemann solver.

References

[1] F. Bouchut, C. Chalons, S. Guisset, *An entropy satisfying two-speed relaxation system for the barotropic Euler equations. Application to the numerical approximation of low Mach number flows.*, Numerische Mathematik **145** (2020), 35–76.

[2] V. Desveaux, M. Zenk, B. Berthon, C. Klingenberg, *Well-balanced schemes to capture non-explicit steady states on the Euler equation with a gravity*, International Journal for Numerical Methods in Fluids **81** (2016), 104–127.

Individual based models for bacterial movement exhibiting Lévy-flight type movement induced by intra-cellular noise

Min Tang

Kinetic-transport models that relate the intra-cellular reaction with the run-and-tumble process are considered as the correct description of microscopic level bacterial movement. Various macroscopic equations of Keller-Segel type or hyperbolic type have been derived from the pathway based kinetic-transport equations for E.coli chemotaxis. Most biological processes have a lot of noise, intrinsic or extrinsic. For E.coli chemotaxis, noise can occurs in the signaling pathways and affects the tumbling rate. We work on an individual-based model and a kinetic equation whose pathways and tumbling kernels are biologically relevant. Super diffusion can arise in the macroscopic limits, under proper scaling and conditions on the tumbling frequency as well as the form of noise. Biologically relevant pathways and tumbling kernels are considered that allows for numerical or possible experimental verifications.

On Landau damping coupled with relaxation for the Vlasov-Poisson-BGK equation for small collision frequencies

Lena Baumann

(joint work with Christian Klingenberg, Marlies Pirner)

When Landau damping was discovered for the Vlasov-Poisson equation in the 1940s in a strictly mathematical way by the Soviet physicist Lev Landau [2] this was a quite astonishing result for the mathematical and physicist community. For the Vlasov-Poisson-BGK equation with small collision frequencies we show, using Landau's approach, that there is an additional damping effect coming from the relaxation.

In a one-dimensional setting the Vlasov-Poisson-BGK equation is given by

$$\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} - \frac{e}{m}\, E \cdot \frac{\partial f}{\partial v} = \lambda\, (M - f), \tag{1}$$

where $f(x, v, t)$ denotes the particle distribution function of electrons with mass m and elementary charge e in a self-consistent electric field E with a neutralising ion background. The collision frequency λ in the BGK operator [1] on the right-hand side is assumed to be small and M is given as the Maxwellian distribution

$$M(x, v, t) = \frac{n(x, t)}{(2\pi T_0/m)^{1/2}} \exp\Big(-\frac{|v - u(x, t)|^2}{2T_0/m}\Big)$$

with $n(x, t) = \int_{\mathbb{R}} f\ dv$ being the macroscopic density and $u(x, t) = \frac{1}{n(x,t)} \int_{\mathbb{R}} fv\ dv$ the macroscopic velocity. Note that the temperature is set to a constant value T_0. Due to Maxwell's equations the electric field is coupled to (1) by

$$\frac{\partial E}{\partial x} = e\, \Big(n_0 - \int_{\mathbb{R}} f\ dv\Big),$$

where n_0 denotes the constant background density of neutralising ions.

We start from a small initial perturbation of the equilibrium function, perform a Fourier expansion in the space and a Laplace transform in the time variable. With this procedure we obtain an expression for the Laplace transform $\tilde{\sigma}$ of the density of the perturbation in the form

$$\tilde{\sigma}(k, \omega) = \frac{N(k, \omega)}{D(k, \omega)}, \tag{2}$$

where the variable k arises from the Fourier expansion and ω from the Laplace transform. The inverse Laplace transform shall then be computed by using the residue theorem. Therefore, we show that for fixed values of k the poles of (2) are exactly the zeros of the denominator and call $D(k, \omega) = 0$ the corresponding dispersion relation.

For examining the zeros of the dispersion relation we first follow a paper by Wood and Ninham [5] and show by analytical means and approximations that the damping effect for the Fourier components of the density σ can be split up into a collisional damping due to the BGK relaxation and a Landau damping part. In a second step we confirm this result numerically using a code provided by E. Sonnendrücker [4].

As an outlook, further studies could be done not just for one species of particles but for the two species model of the Vlasov-Poisson-BGK system introduced in [3].

References

[1] P.L. Bhatnagar, E.P. Gross, M. Krook, *A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-Component Systems*, Physical Review **94**(3) (1954), 511–525.

[2] L. Landau, *On the vibrations of the electronic plasma*, J. Phys. U.S.S.R. **10**(1) (1946), 25–34.

[3] M. Pirner, *Kinetic modelling of gas mixtures*, Würzburg University Press (2018).

[4] E. Sonnendrücker, *Numerical Methods for the Vlasov-Maxwell equations*, Preprint (2019).
[5] W.P. Wood, B.W. Ninham, *Collisional damping of plasma oscillations*, Aust. J. Phys. **22** (1969), 453–458.

Well-balanced treatment of gravity in astrophysical fluid dynamics simulations at low Mach numbers

Philipp V. F. Edelmann

(joint work with Leonhard Horst, Jonas P. Berberich, Robert Andrassy, Johann Higl, Giovanni Leidi, Christian Klingenberg, Friedrich K. Röpke)

Accurate simulations of flows in the interiors of stars are crucial to improving our understanding of stellar structure and evolution. Because the typically slow flows are but tiny perturbations on top of a close balance between gravity and pressure gradient, such simulations place heavy demands on numerical hydrodynamics schemes.

We demonstrate how discretization errors on grids of reasonable size can lead to spurious flows orders of magnitude faster than the physical flow. Well-balanced numerical schemes can deal with this problem.

Three such schemes are applied in the implicit, finite-volume code SLH solving the Euler equations in combination with a low-Mach-number numerical flux function. We compare how the schemes perform in four numerical experiments addressing some of the challenges imposed by typical problems in stellar hydrodynamics.

We find that the α-β [1, 2] and Deviation [3] well-balancing methods can accurately maintain hydrostatic solutions provided that gravitational potential energy is included in the total energy balance. They accurately conserve minuscule entropy fluctuations advected in an isentropic stratification, which enables the methods to reproduce the expected scaling of convective flow speed with the heating rate. The Deviation method also substantially increases accuracy of maintaining stationary orbital motions in a Keplerian disk on long time scales. The Cargo–LeRoux method [4] fares substantially worse in our tests, although its simplicity may still offer some merits in certain situations.

Overall, we find the well-balanced treatment of gravity in combination with low Mach number flux functions essential to reproducing correct physical solutions to challenging stellar slow-flow problems on affordable collocated grids. Further details are found in a recent publication [5].

References

[1] Berberich, J. P., Chandrashekar, P., & Klingenberg, C. 2018, in Theory, Numerics and Applications of Hyperbolic Problems I, Springer Proceedings in Mathematics & Statistics 236, ed. C. Klingenberg & M. Westdickenberg
[2] Berberich, J. P., Chandrashekar, P., Klingenberg, C., & Röpke, F. K. 2019, Communications in Computational Physics
[3] Berberich, J. P., Chandrashekar, P., & Klingenberg, C. 2021, Computers & Fluids, 104858

[4] Cargo, P. & Le Roux, A. 1994, Comptes rendus de l'Académie des sciences. Série 1, Mathématique, 318, 73
[5] Edelmann P. V. F., Horst L., Berberich J. P., Andrassy R., Higl J., Klingenberg C., Roepke F. K., 2021, arXiv, arXiv:2102.13111

Approximate evolution operators for the Active Flux method

Wasilij Barsukow

Hyperbolic conservation laws, such as the Euler equations of compressible hydrodynamics, exhibit a large variety of phenomena, in particular in multiple spatial dimensions. This inherent complexity is reflected in high computational cost associated with attempts of solving the equations numerically. However, often additional difficulties arise because of inefficient or unadapted numerical methods, i.e. methods which require a resolution (in time or space) that is much higher than the desired resolution of the sought numerical solution. It is this latter aspect that is addressed in this work, which focuses on the development of a novel family of numerical methods (*Active Flux*).

With the Cauchy problem being the natural setting for hyperbolic conservation laws, it is customary to integrate the numerical approximations forward in time in an explicit way. This, however, turns out to require *upwinding*, which replaces (unstable) central spatial derivatives by specific one-sided derivatives. The choice of upwind direction traditionally (both for Finite Volume and Finite Element methods, such as Discontinuous Galerkin) involves Riemann solvers, i.e. exact or approximate solutions of initial value problems associated to discontinuous data. Godunov's method proposes to introduce such a discontinuity at every cell interface.

The extension of this strategy to multiple spatial dimensions does not reach up to the success of some finite difference methods (e.g. [MR01, Bar19]) that were obtained by a less fundamental approach, as was shown in [BK20]. These methods (examples of so-called *structure preserving* methods) preserve discrete involutions and discretize all the stationary states of a PDE, instead of keeping stationary discretizations of merely trivial ones. All this is associated with the practical advantage of achieving excellent results on coarse grids. It thus has become clear that there is a large potential of saving computational cost, but a lack of fundamental principles according to which such methods can be derived.

1. The Active Flux method

A promising structure preserving numerical method is the novel Active Flux method ([vL77, ER13]), which presents an alternative to the traditional Godunov idea. It has been initially derived for linear problems, and was shown to be vorticity and stationarity preserving for linear acoustics on Cartesian grids ([BHKR19]). The idea of Active Flux is to reconstruct the solution globally continuously, by introducing additional pointwise degrees of freedom at cell boundaries. It thus is a blend of Finite Volume and Finite Element ideas. The evolution of the cell averages follows trivially from the available data at cell boundaries. The evolution of the

pointwise degrees of freedom, however, does not follow the usual Finite Element approach, which might be in parts the reason behind Active Flux' success.

Finite element (and also finite volume) methods often adapt a method-of-lines approach, separating the spatial discretization from the integration in time. Performing the former, one ends up with a large system of ODEs, which are solved by more or less standard ODE integrators, yielding the latter. On the contrary, in the initial versions of Active Flux, devoted to linear problems, the point values were updated by applying the exact evolution operator to the initial data given by the (piecewise parabolic) continuous reconstruction of the data at the previous time step.

This would mean that the point value $q_{i+\frac{1}{2}}^{n+1}$ at time t^{n+1} is the value $q(t^{n+1} - t^n, x_{i+\frac{1}{2}})$ of an exact evolution $q(t,x)$ of piecewise defined initial data

$$q(0,x) = -3(2\bar{q}_i^n - q_{i-\frac{1}{2}}^n - q_{i+\frac{1}{2}}^n)\frac{(x-x_i)^2}{\Delta x^2} \tag{1}$$

$$+ (q_{i+\frac{1}{2}}^n - q_{i-\frac{1}{2}}^n)\frac{x-x_i}{\Delta x} + \frac{6\bar{q}_i^n - q_{i-\frac{1}{2}}^n - q_{i+\frac{1}{2}}^n}{4} \quad \text{if} \quad x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \tag{2}$$

where $\bar{q}_i^n$ denotes the average of q in cell i at time t^n. Note that

$$q(0, x_{i\pm\frac{1}{2}}) = q_{i\pm\frac{1}{2}}^n \qquad \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(0,x)\,\mathrm{d}x = \bar{q}_i^n \tag{3}$$

For linear advection $\partial_t q + c\partial_x q = 0$, the evolution operator is just $q(t,x) = q(0, x-ct)$, and thus (with the CFL number $\lambda = \frac{c(t^{n+1}-t^n)}{\Delta x}$) one obtains for $c > 0$

$$q_{i+\frac{1}{2}}^{n+1} = -6\bar{q}_i^n(\lambda-1)\lambda + q_{i-\frac{1}{2}}^n\lambda(3\lambda-2) + q_{i+\frac{1}{2}}^n(\lambda-1)(3\lambda-1) \tag{4}$$

$$\bar{q}_i^{n+1} = \bar{q}_i^n - \lambda\frac{q_{i+\frac{1}{2}}^n + 4q_{i+\frac{1}{2}}^{n+\frac{1}{2}} + q_{i+\frac{1}{2}}^{n+1} - q_{i-\frac{1}{2}}^n + 4q_{i-\frac{1}{2}}^{n+\frac{1}{2}} + q_{i-\frac{1}{2}}^{n+1}}{6} \tag{5}$$

which cannot be obviously associated to a spatial discretization and a subsequent application of an ODE solver (compare to examples in [Abg20]).

The advantage of time evolution (4) lies in its immediate stability, ranging up to the physical stability condition of $\lambda \leq 1$, and a natural derivation. Interestingly, it has been shown in [HKS19] that the above method can be given the interpretation of an ADER-type evolution: the formal Taylor series of $q(t,x)$ in time at $x = x_{i+\frac{1}{2}}$ is truncated and the time derivatives replaced by spatial derivatives using the PDE. Whereas the value of q at $x_{i+\frac{1}{2}}$ does exist, the globally continuous reconstruction does not imply the same for derivatives. In [HKS19] it is shown that for linear one-dimensional problems replacing the evaluation of a derivative at the location of its discontinuity by solutions of Riemann problems *in the derivatives* yields exactly the same method (4). However, for nonlinear problems the properties of such an approach are less clear, the equation governing the evolution of derivatives complicated, and the solution of Riemann problems for these (non-conservative) equations, generally unknown.

The work presented here is part of an effort to extend Active Flux to nonlinear problems in a way that stays as close possible to the approach used for linear problems. More precisely, the aim is to find (iterative) approximations to evolution operators, such that they revert to exact evolution operators on linear problems. For example, in case of a scalar nonlinear conservation law, the concept of characteristics persists from the linear case, and hope is that the speed of the characteristic can be estimated to sufficient accuracy. Recent advances for this case, and the case of one-dimensional systems, are presented next.

2. Scalar conservation laws

An approximate evolution operator for scalar conservation laws has been suggested in [Bar21]. Assume for the moment that no shocks are present. For

$$\partial_t q + a(q)\partial_x q = 0 \qquad a\colon \mathbb{R} \to \mathbb{R} \qquad q\colon \mathbb{R}_0^+ \times \mathbb{R} \to \mathbb{R} \tag{6}$$

the characteristic starting at $x = \xi$ at time $t = 0$ is subject to the relation

$$\xi = x - a(q(0, \xi))t \tag{7}$$

which can be solved iteratively:

$$\xi^{(0)} := x \qquad \xi^{(n+1)} := x - a(q(0, \xi^{(n)}))t \tag{8}$$

$\xi^{(n)}$ is approximating ξ to an error $\mathcal{O}(t^{n+1})$ ([Bar21]), and moreover for linear problems, one iteration gives the exact solution.

3. Systems of conservation laws in 1-d

For the case of systems in one spatial dimension the concept of characteristics still persists, but they are curved and, generally speaking, no quantities are constant along any of them. For simplicity, however, assume first that such quantities exist (as is the case for the shallow water equations, for example). Then, a nonlinear $m \times m$ system

$$\partial_t q + J(q)\partial_x q = 0 \qquad q\colon \mathbb{R}_0^+ \times \mathbb{R} \to \mathbb{R}^m \tag{9}$$

can be written as

$$\partial_t Q + \operatorname{diag}(\lambda_1, \ldots, \lambda_m)\partial_x Q = 0 \qquad Q\colon \mathbb{R}_0^+ \times \mathbb{R} \to \mathbb{R}^m \tag{10}$$

where each eigenvalue λ_i of J is considered a function of $Q = (Q_1, \ldots, Q_m)^{\mathrm{T}}$. Thus, Q_i is constant along the i-th characteristic, but the characteristic is curved, as its slope additionally depends on the values of the other variables.

Considering the first two steps of the fixpoint iteration that successfully yielded an approximate evolution operator in the scalar case, one might be tempted to choose ($m = 2$ to save a tree)

$$\tilde{Q}_j(t, x) = Q_{j,0}\Big(x - t\lambda_j(Q_{1,0}(x - t\lambda_j(x)), Q_{2,0}(x - t\lambda_j(x)))\Big) \quad j = 1, 2 \tag{11}$$

as an approximate evolution operator. Here, $Q_{j,0}$ denotes the initial data of Q_j and $\lambda_j(x)$ is short-hand for $\lambda_j(Q_{1,0}(x), Q_{2,0}(x))$. Unfortunately, the error (in t) of this approximation is no better than simply taking

$$\tilde{Q}_j(t,x) = Q_{j,0}\Big(x - t\lambda_j(x)\Big) \tag{12}$$

and not enough to achieve a third order method, as is customary for Active Flux.

This possibly surprising result has to do with the fact that characteristics are curved. It turns out that an approximate operator of sufficient order of accuracy is obtained as follows:

$$\tilde{Q}_j(t,x) = Q_{j,0}\left(x - t\lambda_j\left(Q_{1,0}\left(x - t\frac{\lambda_1(x)+\lambda_j(x)}{2}\right),\right.\right. \tag{13}$$

$$\left.\left. Q_{2,0}\left(x - t\frac{\lambda_2(x)+\lambda_j(x)}{2}\right)\right)\right) \quad j = 1,2 \tag{14}$$

Note how it reduces to the second iteration of operator (8) in the scalar case.

The reason for this is the following. Imposing the evolution operator to have the shape $\tilde{Q}_j(t,x) = Q_{j,0}\Big(x - t\lambda_j^*\Big)$ for some λ_j^* means that the curved characteristic is replaced by a straight characteristic with *average* speed λ^*, which in general is different both from its speed at the footpoint and at time t. Thus,

$$\lambda_j^* \simeq \frac{1}{t}\int_0^t \lambda_j\Big(Q_1(\tau, X_j(\tau)), \ldots, Q_m(\tau, X_j(\tau))\Big)\mathrm{d}\tau \tag{15}$$

where $X_j\colon \mathbb{R}_0^+ \to \mathbb{R}$ denotes the j-th characteristic curve. It is not surprising (and is proved to be true in [Bar21]) that a good estimate therefore is

$$\lambda_j^* \simeq \lambda_j\left(Q_1\left(\frac{t}{2}, X_j\left(\frac{t}{2}\right)\right), \ldots, Q_m\left(\frac{t}{2}, X_j\left(\frac{t}{2}\right)\right)\right) \tag{16}$$

and

$$Q_i\Big(\frac{t}{2}, X_j\Big(\frac{t}{2}\Big)\Big) \simeq Q_i\Big(\frac{t}{2}, x - \frac{t}{2}\lambda_j(x)\Big) \simeq Q_{i,0}\Big(x - t\frac{\lambda_i(x)+\lambda_j(x)}{2}\Big) \tag{17}$$

which is the expression stated earlier.

For systems without characteristic variables (such as the Euler equations) similar approximate evolution operators can be found. In that case, not only the characteristic speeds need to be approximated, but also the transformation matrix that diagonalizes J. For details, see [Bar21].

Both for scalar problems and for systems it is necessary to anticipate the case of crossing characteristics, and thus shock formation. Because of global continuity of the reconstruction, a shock does not form instantaneously, and often enough, the CFL condition imposes a smaller time step than the shock formation time. In other cases, it is suggested in [Bar21] to compute several estimates of possible characteristics, and select one of them.

4. Outlook

Future work will be devoted to the multi-dimensional case. There, the additional difficulty is the conceptual replacement of characteristic lines by characteristic cones. This means that predictor-corrector strategies are not only needed to approximate the speed (i.e. the tangent to the cone), but also the directions.

References

[Abg20] Rémi Abgrall. A combination of residual distribution and the active flux formulations or a new class of schemes that can combine several writings of the same hyperbolic problem: application to the 1d euler equations. *arXiv preprint arXiv:2011.12572*, 2020.

[Bar19] Wasilij Barsukow. Stationarity preserving schemes for multi-dimensional linear systems. *Mathematics of Computation*, 88(318):1621–1645, 2019.

[Bar21] Wasilij Barsukow. The active flux scheme for nonlinear problems. *Journal of Scientific Computing*, 86(1):1–34, 2021.

[BHKR19] Wasilij Barsukow, Jonathan Hohm, Christian Klingenberg, and Philip L Roe. The active flux scheme on Cartesian grids and its low Mach number limit. *Journal of Scientific Computing*, 81(1):594–622, 2019.

[BK20] Wasilij Barsukow and Christian Klingenberg. Exact solution and a truly multidimensional Godunov scheme for the acoustic equations. *submitted, preprint available as arXiv:2004.04217*, 2020.

[ER13] Timothy A Eymann and Philip L Roe. Multidimensional active flux schemes. In *21st AIAA computational fluid dynamics conference*, 2013.

[HKS19] Christiane Helzel, David Kerkmann, and Leonardo Scandurra. A new ADER method inspired by the active flux method. *Journal of Scientific Computing*, 80(3):1463–1497, 2019.

[MR01] Keith William Morton and Philip L Roe. Vorticity-preserving Lax-Wendroff-type schemes for the system wave equation. *SIAM Journal on Scientific Computing*, 23(1):170–192, 2001.

[vL77] Bram van Leer. Towards the ultimate conservative difference scheme. IV. A new approach to numerical convection. *Journal of computational physics*, 23(3):276–299, 1977.

Statistical solutions to the barotropic Navier-Stokes system

Eduard Feireisl

(joint work with F. Fanelli)

We introduce a new concept of statistical solution in the framework of weak solutions to the barotropic Navier–Stokes system with inhomogeneous boundary conditions. Statistical solution is a family of Markov operators on the set of probability measures on the data space containing the initial and the boundary data. The operators enjoy the following properties: 1. Semiflow (semigroup) property 2. The solution is deterministic for deterministic data 3. Continuity in a suitable Bregman-Wasserstein metric.

Convex integration applied to the compressible Euler equations

Simon Markfelder

The question of well-posedness for the compressible Euler equations has been answered quite satisfactory in *one* space dimension. But in *multiple* space dimensions it has been shown in past 10 years, that solutions are not unique in the class of bounded weak entropy solutions. These non-uniqueness results are achieved using a technique called *convex integration*, which was developed by Gromov and first used in the context of fluid flow equations by De Lellis and Székelyhidi [2].

To apply this method, one proceeds as follows. First one replaces all nonlinearities by new unknowns. More precisely the barotropic compressible Euler equations

$$\begin{aligned} \partial_t \varrho + \operatorname{div} \mathbf{m} &= 0, \\ \partial_t \mathbf{m} + \operatorname{div} \left(\frac{\mathbf{m} \otimes \mathbf{m}}{\varrho} + p(\varrho) \right) &= \mathbf{0}, \end{aligned} \tag{1}$$

with unknown density ϱ and momentum $\mathbf{m}$, are rewritten as

$$\begin{aligned} \partial_t \varrho + \operatorname{div} \mathbf{m} &= 0, \\ \partial_t \mathbf{m} + \operatorname{div} (\mathbb{U} + q\mathbb{I}) &= \mathbf{0}, \end{aligned} \tag{2}$$

where $\mathbb{U}$ and q are additional unknown functions which take values in the symmetric traceless matrices and in $\mathbb{R}$, respectively. Instead of solving (1) one can equivalently look for solutions of the underdetermined linear system (2) which take values in the set

$$K := \left\{ (\varrho, \mathbf{m}, \mathbb{U}, q) \,\middle|\, \mathbb{U} + q\mathbb{I} = \frac{\mathbf{m} \otimes \mathbf{m}}{\varrho} + p(\varrho) \right\}.$$

Now a *subsolution* is defined as a solution of the linear system (2) which takes values in the Λ-convex hull K^Λ of the set K. Roughly speaking convex integration is a method which forms subsolutions into solutions by adding plane wave oscillations.

With this method at hand, it suffices to find an appropriate subsolution if one wants to solve (1). In particular, convex integration becomes a powerful tool if the class of possible subsolutions is large, i.e. if K^Λ is much larger than K.

In this talk we explain two existing convex integration approaches for the compressible Euler equations (1) and, in addition to that, some ideas of a possible new approach:

(1) The first approach goes back to Feireisl [3] and Chiodaroli [1]. Here the basic idea is to consider the density ϱ as well as q only as parameters which are fixed a priori and which are not determined by convex integration. This way one has been able to construct solutions which even satisfy the energy inequality. However this approach seems to have two weak points:
   (a) The fact that ϱ and q are merely parameters might restrict the class of possible subsolutions.
   (b) The energy inequality represents another restriction on the class of possible subsolutions.

(2) This approach can be found in the speaker's PhD Thesis [4] and tackles weak point (a). To this end we let ϱ and q be part of the game, i.e. they are determined by convex integration, too. However this does *not* lead to a larger class of possible subsolutions. Furthermore using this approach there is no way to achieve solutions which satisfy the energy inequality.
(3) The third approach is work in progress and shall tackle weak point (b). In this talk we present our current state.

References

[1] E. Chiodaroli, *A counterexample to well-posedness of entropy solutions to the compressible Euler system*, J. Hyperbolic Differ. Equ. **11**(3) (2014), 493–519.
[2] C. De Lellis and L. Székelyhidi Jr., *On admissibility criteria for weak solutions of the Euler equations*, Arch. Ration. Mech. Anal. **195**(1) (2010), 225–260.
[3] E. Feireisl, *Maximal dissipation and well-posedness for the compressible Euler system*, J. Math. Fluid Mech. **16** (2014), 447–461.
[4] S. Markfelder, *Convex Integration Applied to the Multi-Dimensional Compressible Euler Equations*, PhD-Thesis (2020), available on arXiv: 2001.04373.

On convergence of the invariant domain preserving scheme by Jean-Luc Guermond and Bojan Popov to a dissipative measure-valued solution in the case of the complete Euler equations

Eva Horlebein

(joint work with Eduard Feireisl, Christian Klingenberg, Simon Markfelder)

Finding a suitable notion of solution is one of the fundamental problems when dealing with Euler equations and hyperbolic partial differential equations in general. While it could be shown that in one space dimension weak solutions provide an appropriate solution concept, in multiple dimensions the situation is much more complex. The groundbreaking development in this field was the introduction of measure-valued solutions by R. DiPerna [5] in 1985. Recently, a refined version of this solution concept was proposed: the dissipative measure-valued solutions, see e.g. [3] for the complete Euler equations. In contrast to measure-valued solutions, dissipative measure-valued solutions are required to satisfy an entropy inequality as additional admissibility criterion. Using this notion of solution, our aim is to prove the convergence of the numerical scheme proposed by J.-L. Guermond and B. Popov in [1] in the case of compressible Euler equations.

The scheme under consideration uses a finite element approach to compute solutions of general hyperbolic systems. It's special property is that (under a positivity assumption on the reference shape functions and a CFL condition) every convex invariant set containing the initial data and it's approximation is an invariant domain for this scheme [1]. That is, in every computation step the numerical solution and its finite element approximation coefficients remain in the convex invariant set B if the initial data and its approximation and corresponding coefficients lie in B. Note that in this context invariant sets are only defined for Riemann problems with a unique solution which has a finite speed of propagation.

Now, our aim is to proof the convergence of this numerical scheme to a dissipative measure-valued solution in the case of the compressible Euler equations. The exact definition we use for such solutions is given in [2].

The reason dissipative measure-valued solutions are a suitable concept of solution for the compressible Euler equations is that they satisfy a weak-strong uniqueness property, as was shown in [4] and [3]. That is, if there is a strong solution to some initial data, the dissipative measure-valued solution to this data coincides with the strong solution on its life span.

The procedure of the proposed proof is adapted from related proofs found in [2] and [3]. The general idea is to first establish suitable a priori bounds for the conserved quantities to show that the approximating sequence contains a subsequence that converges to some limit and in a second step prove the consistency of the scheme. This way, when taking the limit of the consistency equations the convergence (of a subsequence) to a dissipative measure-valued solution follows from the fundamental property of Young measures.

Note, that while we have already proven suitable a priori bounds by exploiting the invariant domain preserving property of the method, proving the consistency of the scheme is currently work in progress. Also note, that to reach arbitrary times we will need to ensure that the size of each time step does not approach zero by meeting the CFL condition. So far it is not clear how this can be achieved except by assuming it.

References

[1] J.-L. Guermond, B. Popov, *Invariant Domains and First-Order Continuous Finite Element Approximation for Hyperbolic Systems*, SIAM J. Numer. Anal. **54(4)** (2016), 2466–2489.

[2] E. Feireisl, M. Lukáčová-Medvid'ová, H. Mizerová, *Convergence of Finite Volume Schemes for the Euler Equations via Dissipative Measure-Valued Solutions*, Foundations of Computational Mathematics **20** (2020), 923–966.

[3] J. Březina, E. Feireisl, *Measure-valued solutions to the complete Euler system*, J. Math. Soc. Japan **70(4)** (2018), 1227–1245.

[4] P. Gwiazda, A. Świerczewska-Gwiazda, E. Wiedemann, *Weak-strong uniqueness for measure-valued solutions of some compressible fluid models*, Nonlinearity **28(11)** (2015), 3873–3890.

[5] R. J. DiPerna, *Measure-valued solutions to conservation laws*, Arch. Rational Mech. Anal. **88** (1985), 223–270.

Introduction to Inverse Problems and Transport Equations I and II

Ru-Yu Lai

(joint work with Qin Li, Gunther Uhlmann, and Yang Yang)

In these two talks, we first introduce inverse problems and their related mathematical backgrounds. We then report our work concerned with the asymptotic limit of the radiative transfer equation (RTE). Finally, the reconstruction of the collision kernel in nonlinear Boltzmann equation is presented.

Inverse problems play an essential role in modern scientific inquiries. They are the *inverse* to the classical direct problems. While one aims to find the unique effect (solution) of a given cause in the direct problems, the inverse problems can be interpreted as finding the cause of a given effect or specifying the model from certain given information of effect. The goals of inverse problems involve the reconstruction of the internal characteristics of an inaccessible region from the boundary measurements as well as the determination of coefficients appearing in the underlying equations from the input and output measurements.

A prototypical example of such problems is the Calderón problem, known as the electrical impedance tomography, which is a medical imaging technique for reconstructing the electrical conductivity inside a body by using voltage and current measurements at the boundary. Since Calderón proposed this problem in 1980 [2], it has received great attention and been intensively studied in the literature [5]. The Calderón problem is mathematically modeled as follows. For a given voltage potential h on the boundary, the electrical potential u in the body $\Omega \subset \mathbb{R}^n$ is governed through the conductivity equation:

$\nabla \cdot (\gamma \nabla u) = 0$ in Ω and $u = h$ on $\partial\Omega$, where γ is the unknown conductivity.

The Calderón problem is to determine γ in Ω from the Dirichlet-to-Neumann (DN) map defined by $\Lambda_\gamma h := \gamma \frac{\partial u}{\partial \nu}\big|_{\partial\Omega}$, with ν is the unit outer normal vector to the boundary $\partial\Omega$.

Several aspects of inverse problems are interesting in the mathematical theory and practical applications, including: 1) Uniqueness: does the given data uniquely determine the unknown? 2) Stability: is the reconstruction of the unknown sensitive to measurement errors in the data? 3) Reconstruction formula: can the unknown be explicitly expressed by a formula depending only on the given data?

The radiative transfer equation in the diffusion regime. We consider the connection between the inverse problem for the RTE and the inverse problem for the elliptic equation.

The model for describing the dynamics of photon particles in a medium can be described by the stationary RTE (linear Boltzmann equation):

$$\begin{cases} v \cdot \nabla_x f + (K_n \sigma + K_n^{-1} k)(x) f = K_n^{-1} k(x) \int_{\mathbb{S}^{n-1}} f(x, v') dv', \quad (x, v) \in \Omega \times \mathbb{S}^{n-1}, \\ f|_{\Gamma_-} = \text{given data}, \end{cases}$$

where the sets of incoming and outgoing conditions, Γ_- and Γ_+, are defined by

$$\Gamma_\pm = \{(x, v) \in \partial\Omega \times \mathbb{R}^n : \pm n_x \cdot v > 0\}$$

and n_x is the outward unit normal vector at point x on the boundary $\partial\Omega$. Here the scaling K_n (Knudsen number) is related to the mean distance that takes particles to significantly change direction due to scattering. The inverse problem here is to determine optical properties (absorption and scattering coefficients, σ and k) from the measurements collected from the surface of the medium by illuminating the medium at different positions x on the boundary with various directions v. The boundary measurement is mathematically described by the *albedo* operator:

$$\mathcal{A} : f|_{\Gamma_-} \to f|_{\Gamma_+},$$

which maps from the incoming photon density $f|_{\Gamma_-}$ to the outgoing density $f|_{\Gamma_+}$.

How is the well-posedness of the RTE being deteriorated in the diffusion limit? When the scattering becomes dominant in the diffusion regime ($K_n \ll 1$), the initial direction of the particles is lost due to the multiple interactions with the underlying medium. As a result, the RTE is well-approximated by the diffusion equation as $K_n \to 0$. Note that the inverse problem for the diffusion equation is to recover the optical parameters from the DN map. Unlike the inverse problem for the RTE, this is known to be severely ill-posed and has logarithmic stability estimate [1, 5].

We study the stability estimate of the parameter for the RTE and make its dependence on K_n explicitly [3]. We show that despite the stability is Hölder like, its coefficient blows up in an exponential fashion for small K_n. The derived estimate provides an evidence that reveals the severe ill-posedness could occur when the RTE is in the diffusion regime.

More specifically, let $\mathcal{A}_1$ and $\mathcal{A}_2$ be the albedo operators corresponding to parameters (σ_1, k_1) and (σ_2, k_2), respectively. The following stability estimates were obtained in [3].

Theorem 1.([3]) *Let Ω be a bounded open convex set in $\mathbb{R}^n$, $n = 2, 3$ with C^1 boundary $\partial\Omega$, and let $0 < K_n < 1$. If $K_n < |\log(\|\mathcal{A} - \tilde{\mathcal{A}}\|_*)|^{-\alpha}$ for some $\alpha > 0$, then*

$$\|\sigma_1 - \sigma_2\|_{L^\infty} \leq CK_n^{-3} |\log(\|\mathcal{A}_1 - \mathcal{A}_2\|_*)|^{-\alpha} + CK_n^{-2+\theta} e^{C\theta {K_n}^{-1}} \|\mathcal{A}_1 - \mathcal{A}_2\|_*^\theta,$$

and

$$\|k_1 - k_2\|_{L^\infty} \leq CK_n |\log(\|\mathcal{A}_1 - \mathcal{A}_2\|_*)|^{-\alpha} + CK_n^\theta e^{C\theta {K_n}^{-1}} \|\mathcal{A}_1 - \mathcal{A}_2\|_*^\theta,$$

for some $\theta \in (0, 1)$, $\alpha > 0$, and some positive constant C, independent of K_n, where $\|\cdot\|_*$ is the operator norm from $L^1(\Gamma_-, d\xi)$ to $L^1(\Gamma_+, d\xi)$.

In particular, these estimates connect Hölder stability to Logarithmic stability with explicit dependence on K_n provided that K_n is sufficiently small. The numerical examples in [3] also agree with the above theoretical result.

Reconstruction of collision kernel in nonlinear Boltzmann equation. In [4], we consider an inverse problem for the Boltzmann equation with nonlinear collision operator in dimensions $n \geq 2$.

Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with smooth boundary $\partial\Omega$ with $n \geq 2$. We consider the following Boltzmann equation:

$$\begin{cases} v \cdot \nabla_x F = Q(F,F) & \text{in } \Omega \times \mathbb{R}^n, \\ F = g & \text{on } \Gamma_-, \end{cases} \tag{1}$$

where $F(x,v)$ is the distribution function that depends on the position $x \in \Omega$ and the velocity $v \in \mathbb{R}^n$. The collision operator takes the form

$$Q(H_1, H_2) := \int_{\mathbb{R}^n} \int_{\mathbb{S}^{n-1}} B(v,u,\omega)[H_1(x,u')H_2(x,v') - H_1(x,u)H_2(x,v)]\, d\omega du,$$

where $B(v,u,\omega)$ is the collision kernel and the vectors are related by

$$u' = u - [(u-v)\cdot\omega]\omega \quad \text{and} \quad v' = v + [(u-v)\cdot\omega]\omega.$$

We also denote the boundary operator $\mathcal{A}$ by

$$\mathcal{A} : F|_{\Gamma_-} \mapsto F|_{\Gamma_+}.$$

We show that the kinetic collision kernel can be uniquely determined from the incoming-to-outgoing mappings on the boundary of the domain provided that the kernel satisfies a monotonicity condition.

Theorem 2. ([4]) *Let $\mathcal{A}_j$ be the boundary operator of the problem* (1) *with the kernel B replaced by B_j for $j = 1, 2$. Suppose that*

$$\mathcal{A}_1(g) = \mathcal{A}_2(g)$$

for all $g \in C(\Gamma_-)$ with $\|g\|_{C(\Gamma_-)} < \varepsilon$, where ε is a sufficiently small number. If $B_1 \geq B_2$ pointwisely in $\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{S}^{n-1}$ (Monotonicity condition), then

$$B_1 = B_2 \quad \text{in } \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{S}^{n-1}.$$

To recover the collision kernel, we apply the higher-order linearization technique to the nonlinear Boltzmann equation (1). This technique employs nonlinearity as a tool in solving inverse problems for nonlinear equations. More specifically, we differentiate the nonlinear equation with respect to small parameters to earn simpler linearized equations. Indeed the first linearization leads to the transport equation $v \cdot \nabla_x V = 0$ with data $V = g$ on Γ_-, which is totally irrelevant to collision kernel. The unknown kernel only appears in the source term S of the second linearization $v \cdot \nabla_x W = S$ of (1) with trivial data $W = 0$ on Γ_-, where S is an integral consisting of collision kernel B and the solutions V. Finally, due to plenty of freedom to choose the solutions V, we thus can extract the information of B out of the source term S.

References

[1] G. Alessandrini, *Stable determination of conductivity by boundary measurements*, Appl. Anal., **27** (1988), 153–172

[2] A. Calderón, *On an inverse boundary value problem*, Seminar in Numerical Analysis and its Applications to Continuum Physics (Río de Janeiro: Soc. Brasileira de Matemática), (1980), 65–73

[3] R.-Y. Lai, Q. Li and G. Uhlmann, *Inverse problems for the stationary transport equation in the diffusion scaling*, SIAM Applied Mathematics, **79(6)** (2019), 2340–2358.

[4] R.-Y. Lai, G. Uhlmann and Y. Yang, *Reconstruction of the collision kernel in the nonlinear Boltzmann equation*, SIAM J. Math. Anal. (to appear).
[5] G. Uhlmann, *Electrical impedance tomography and Calderón's problem*, Inverse problems, **25(12)** (2009), 123011.

Shakhov model near a global Maxwellian

Gi-Chan Bae
(joint work with Seok-Bae Yun)

In this talk, we consider the Shakhov model which is a Prandtl number generalization of the Boltzmann-BGK model. More precisely, we construct the global-in-time classical solution of the Shakhov model when the system starts with the initial data near a global Maxwellian. The Prandtl number dependency of the Shakhov operator produces the following dichotomy of the coercivity estimate: When $Pr > 0$, the degeneracy of the linearized Shakhov model is just 5-dimension. But when $Pr = 0$, the kernel of a linear term is 8-dimension having 3-rd order moments of f. So that $Pr = 0$ induces more degeneracy. We overcome the greater degeneracy by obtaining a full coercivity estimate.

The Boltzmann equation is a cornerstone of the rarefied kinetic theory which describes the transport and collision nature of the dynamics of particles. This allowed us to describe the dynamics of gas outside the continuum regime. However, since the Boltzmann equation has a too large numeric cost because of the collision operator, Its relaxation model, the BGK equation, is proposed in [1].

$$\partial_t F + v \cdot \nabla_x F = \mathcal{M}(F) - F,$$

where $\mathcal{M}(F)$ is given by

$$\mathcal{M}(F) = \frac{\rho(x,t)}{\sqrt{2\pi T(x,t)}^3} \exp\left(-\frac{|v - U(x,t)|^2}{2T(x,t)}\right).$$

The macroscopic mass, momentum, temperature are defined as

$$\begin{aligned}
\rho(x,t) &= \int_{\mathbb{R}^3} F(x,v,t)dv, \\
U(x,t) &= \frac{1}{\rho}\int_{\mathbb{R}^3} F(x,v,t)vdv, \\
T(x,t) &= \frac{1}{3\rho}\int_{\mathbb{R}^3} F(x,v,t)|v - U(x,t)|^2 dv.
\end{aligned}$$

The BGK model just shifts the collision operator of the Boltzmann equation by local equilibrium minus F. Nevertheless, the BGK model satisfies important physical features such as conservation laws and H-theorem. Furthermore, the numerical aspect of the BGK model is similar to the Boltzmann equation. However, there is one major defect in the BGK model, which is that the Prandtl number of the BGK model does not fit real monatomic gas. The Prandtl number of the monatomic gas is 2/3 but the Prandtl number of the BGK model computed by

the Chapman-Enskog expansion is 1. The Prandtl number is a physical constant that characterizes matter.

$$Pr = \frac{\text{viscosity}}{\text{thermal conductivity}}.$$

There was two major suggestion to overcome this defects. The first one is the Ellipsoidal BGk model which modified the stress tensor on the BGK operator:

$$\partial_t F + v \cdot \nabla_x F = \frac{1}{1-\nu} \left(\mathcal{M}_\nu(F) - F \right),$$

where

$$\mathcal{M}_\nu(F) = \frac{\rho}{\sqrt{\det(2\pi \mathcal{T}_\nu)}} \exp\left(-\frac{1}{2}(v-U)^T \mathcal{T}_\nu^{-1}(v-U) \right).$$

As we can see, the ES-BGK operator $\mathcal{M}_\nu(F)$ is non-negative, so that the solution of the ES-BGK model also non-negative. The H-theorem also holds.
The other is Shakhov model [6] which modified the heat flux from the BGK model.

$$\partial_t F + v \cdot \nabla_x F = \mathcal{S}(F) - F,$$

where

$$\mathcal{S}(F) = \frac{\rho}{\sqrt{2\pi T}^3} \exp\left(-\frac{|v-U|^2}{2T} \right) \left[1 + \frac{1-Pr}{5} \frac{q \cdot (v-U)}{\rho T^2} \left(\frac{|v-U|^2}{2T} - \frac{5}{2} \right) \right],$$

and the Prandtl number Pr is a non-negative constant. The heat flux q is defined as

$$q(x,t) = \int_{\mathbb{R}^3} F(x,v,t)(v - U(x,t))|v - U(x,t)|^2 dv.$$

By the structure of the Shakhov model, the Shakhov operator $\mathcal{S}(F)$ can take a negative value. So that the mild solution of the Shakhov operator can be negative. Moreover, the Shakhov model satisfies H-theorem only when the F is sufficiently close to the global equilibrium. Despite these defects, since the Shakhov model has the advantage of being more fit in a tough condition, it is widely used in physics and engineering [2, 5, 7, 8]. We consider the classical solution of the Shakhov model when the initial data is close to the global equilibrium.

The general way to study the kinetic equation near a global equilibrium is done through the linearization of equations. In the case of the Boltzmann equation, if we substitute $F = m + \sqrt{m} f$ on the Boltzmann equation, where

$$m(v) = \frac{1}{\sqrt{2\pi}^3} e^{-\frac{|v|^2}{2}},$$

then we have

$$\partial_t f + v \cdot \nabla_x f = Lf + \Gamma(f,f).$$

Then we can derive the following coercivity estimate for the linear term Lf.

$$\langle Lf, f \rangle_{L^2_v} \leq -\delta \| (I-P) f \|^2_{L^2_\nu},$$

where Pf is projection operator onto $\{\sqrt{m}, v\sqrt{m}, |v|^2\sqrt{m}\}$. But this inequality does not give sufficient exponential decay of the L^2 energy norm since it has degeneracy as much as Pf. In spatial torus, substituting macro-micro decomposition $f = Pf + (I-P)f$ on the linearized equation, and applying the Poincaré inequality, we can obtain the following full coercivity estimate [3, 4]:

$$\sum_{|\alpha|\le N} \langle L\partial^\alpha f, \partial^\alpha f\rangle_{L^2_{x,v}} \le -\delta \sum_{|\alpha|\le N} \|\partial^\alpha f\|^2_{L^2_{x,v}}.$$

On the BGK model, we can derive similar linearized equation [9]:

$$\partial_t f + v\cdot\nabla_x f = P_c f - f + \Gamma(f,f),$$

where $P_c f$ is a orthonormal projection spanned by $\{\sqrt{m}, v\sqrt{m}, |v|^2\sqrt{m}\}$. The orthonormal property of P_c guarantees the following equality:

$$\langle Lf, f\rangle_{L^2_v} = -\|(I-P)f\|^2_{L^2_v}.$$

Since the Shakhov operator $\mathcal{S}(F)$ depends on the heat flux q, It also depends on the second moments and third moments of F. So that we should linearize the Shakhov operator by the 13 macroscopic variables (ρ, U, Θ, q). Then we can have the following linearized Shakhov model:

$$\partial_t f + v\cdot\nabla_x f = P_{Pr} f - f + \Gamma(f,f).$$

where

$$P_{Pr} f = P_c f + (1-Pr)P_{nc} f.$$

The projection operator P_{nc} is orthonormal projection related to $v|v|^2$.

Because of the third-order moment term in P_{nc}, depending on the Prandtl number, there occurs dichotomy on the degeneracy. When $Pr > 0$, we have

$$KerL = span\{\sqrt{m}, v\sqrt{m}, |v|^2\sqrt{m}\},$$

and

$$\langle L_{Pr} f, f\rangle_{L^2_{x,v}} \le -\min\{Pr, 1\}\|(I-P_c)f\|^2_{L^2_{x,v}}.$$

On the other hand, $Pr = 0$ yields

$$KerL = span\{\sqrt{m}, v\sqrt{m}, |v|^2\sqrt{m}, v|v|^2\sqrt{m}\},$$

and

$$\langle L_{Pr} f, f\rangle_{L^2_{x,v}} = -\|(I-P_c-P_{nc})f\|^2_{L^2_{x,v}}.$$

Thus we can see that the coercivity estimate of the latter case is more degenerate.

In spatially torus case, the degeneracy on the former case can be recovered by the macro-micro decomposition $f = Pf + (I-P)f$ and Poincaré inequality as in [3, 4]. However, the zero-Prandtl number case has to overcome as much degree as $v|v|^2$. The main problem is that the integration with respect to $(1, v, |v|^2)dv$ has conservation, but the integration with respect to $v|v|^2$ does not conserved.

Therefore, if we give an assumption on the third-order moments of the initial data,

$$\int_{\mathbb{T}^3\times\mathbb{R}^3} F_0(x,v)v|v|^2 dvdx = 0,$$

then we can have the following modified full coercivity estimate:

$$\sum_{|\alpha|\le N} \langle L\partial^\alpha f, \partial^\alpha f\rangle_{L^2_{x,v}} \le -\delta \sum_{|\alpha|\le N} \|\partial^\alpha f\|^2_{L^2_{x,v}} + C\mathcal{E}^2(t).$$

This is joint work with Prof. Seok-Bae Yun, and we are preparing for the submission.

References

[1] Bhathnagor, P., Gross, E. and Krook, M.: A model for collision processes in gases. Physical Review, **94** (1954), no. 3, 511.

[2] Cai, Z., Li, R., Qiao, Z. . NR xx simulation of microflows with Shakhov model. SIAM Journal on Scientific Computing, **34** (2012), no.1, A339–A369.

[3] Guo, Y.: The Vlasov-Maxwell-Boltzmann system near Maxwellians. Invent. Math. **153** (2003), no. 3, 593–630.

[4] Guo, Y.: The Vlasov-Poisson-Boltzmann system near Maxwellians. Comm. Pure Appl. Math. **55** (2002), no. 9, 1104–1135.

[5] Pantazis, S., Valougeorgis, D.: Heat transfer through rarefied gases between coaxial cylindrical surfaces with arbitrary temperature difference. European Journal of Mechanics-B/Fluids, **29** (2010), no. 6, 494–509.

[6] Shakhov, E. M.: Generalization of the Krook kinetic relaxation equation. Fluid dynamics, **3** (1968), no. 5, 95–96.

[7] Titarev, V. A.: Conservative numerical methods for model kinetic equations. Comput. Fluids **36** (2007), no. 9, 1446–1459.

[8] Todorova, B., Steijl, R.: Derivation and numerical comparison of Shakhov and ellipsoidal statistical kinetic models for a monoatomic gas mixture. Eur. J. Mech. B Fluids **76** (2019), 390–402.

[9] Yun, S.-B.: Cauchy problem for the Boltzmann-BGK model near a global Maxwellian. J. Math. Phys. **51** (2010), no. 12, 123514, 24 pp.

Numerical schemes for multi-species (quantum) BGK equations

Sandra Warnecke

(joint work with Christian Klingenberg, Marlies Pirner)

We consider a (space homogeneous) kinetic model of a gas mixture. Each species is described by a BGK model, where for N species we have N BGK terms for each species, describing the pairwise interaction of each species with every other. Due to illustration purposes we restrict to two species in this talk, but everything goes through for an arbitrary number of different kinds of species since only binary interactions are taken into account.

Let $f_1 = f_1(\mathbf{p}, t), f_2 = f_2(\mathbf{p}, t) > 0$ for $\mathbf{p} \in \mathbb{R}^3$ and $t \geq 0$. The model is given by the equations

$$\partial_t f_1 = (A_{11,\tau(1)} - f_1) + (A_{12,\tau(1)} - f_1)$$
$$\partial_t f_2 = (A_{22,\tau(2)} - f_2) + (A_{21,\tau(2)} - f_2)$$

with the attractors

$$A_{ii,\tau(i)}(\mathbf{p}, t) = \frac{1}{\exp\left(m_i a_i |\frac{\mathbf{p}}{m_i} - \mathbf{b}_i|^2 + c_i\right) + \tau(i)}$$
$$A_{ij,\tau(i)}(\mathbf{p}, t) = \frac{1}{\exp\left(m_i a |\frac{\mathbf{p}}{m_i} - \mathbf{b}|^2 + c_{ij}\right) + \tau(i)}$$

and $\tau(i) \in \{-1, 0, +1\}$ which specifies whether the particles are chosen to be classic ($\tau = 0$), fermions ($\tau = -1$) or bosons ($\tau = +1$). This model covers both a special case of a pure classic gas mixture presented in [1] and a pure quantum gas mixture presented in [2]. Additionally, we extend the model to allow for a mixture of quantum and classic particles. With the same strategy as in [2] we can show (under some integrability conditions) that there exist unique parameters $a_1, a_2, a \in \mathbb{R}^+$, $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b} \in \mathbb{R}^3$ and $c_1, c_2, c_{12}, c_{21} \in \mathbb{R}$ such that mass, total momentum and total energy are conserved. Moreover, an $\mathcal{H}$-theorem can be proven, and we have analytic rates which describe the time decay of the differences between the mean velocities and the temperatures of the two species.

We design a numerical method where the right hand side of the equations is treated implicitely. This means that the values of the attractors at the next time step are needed for an update of the distribution functions. Inspired by the proofs in [3] we determine these values by the minimization of a specific Lagrange functional. By this approach the conservation properties are automatically fulfilled at the discrete level and for all time steps.

We show numerical results for a pure classic gas mixture, for a pure fermion gas mixture and for a mixture of classic and fermion particles.

References

[1] C. Klingenberg, M. Pirner, G. Puppo, *A consistent kinetic model for a two-component mixture with an application to plasma*, Kinetic and Related Models Vol. 10, No. 2, pp. 445–465 (2017)

[2] G.-C. Bae, C. Klingenberg, M. Pirner, S.-B. Yun, *BGK Model of the multi-species Uehling-Uhlenbeck equation*, Kinetic and Related Models (2021) 14 (1) : 25–44

[3] J. Haack, C. Hauck, C. Klingenberg, M. Pirner, S. Warnecke *A consistent BGK model with velocity-dependent collision frequency for gas mixtures*, submitted (2021), arXiv:2101.09047

Ergodic theory for energetically open compressible fluid flows

Eduard Feireisl
(joint work with F. Fanelli, M. Hofmanova)

The ergodic hypothesis is examined for energetically open fluid systems represented by the barotropic Navier-Stokes equations with general inflow/outflow boundary conditions. We show that any globally bounded trajectory generates a stationary statistical solution, which is interpreted as a stochastic process with continuous trajectories supported by the family of weak solutions of the problem. The abstract Birkhoff–Khinchin theorem is applied to obtain convergence (in expectation and a.s.) of ergodic averages for any bounded Borel measurable function of state variables associated to any stationary solution. Finally, we show that validity of the ergodic hypothesis is determined by the behavior of entire solutions In particular, the ergodic averages converge for any trajectory provided its omega-limit set in the trajectory space supports a unique (in law) stationary solution.

Low rank structure in the forward and inverse kinetic theory

Qin Li
(joint work with Ke Chen, Shi Chen, Christian Klingenberg, Ru-Yu Lai, Jianfeng Lu, Gunther Uhlmann, Stephen Wright)

Kinetic theory is a body of theory from statistical mechanics. It is useful in describing the dynamics of a large number of particles, but its high dimensional structure makes the computation infeasible. In multi-scale regimes, however, kinetic equations can be compressed: The Boltzmann equation is asymptotically equivalent to the Euler equations, and the radiative transfer equation is asymptotically equivalent to the diffusion equation. In linear algebra, this phenomenon is equivalent to a system being of low rank.

I will discuss how the low rank structure forms, and how it affects the computation. In the forward regime, inserting the low-rank structure greatly advances the computation, but in the inverse regime, the system being of low rank typically makes the problems significantly harder.nd large space scale simulations to approach the macroscopic scales. A highly accurate deduced equation of state for the Euler equations establishes a one-to-one correspondence of the molecular dynamics and the continuum solutions.

References

[1] Christian Klingenberg, Ru-Yu Lai, and Qin Li, *Reconstruction of the Emission Coefficient in the Nonlinear Radiative Transfer Equation*, SIAM J. Appl. Math. **81(1)** (2021), 91-106.
[2] Ru-Yu Lai, Qin Li and Gunther Uhlmann, *Inverse Problems for the Stationary Transport Equation in the Diffusion Scaling*, SIAM J. Appl. Math. **79(6)** (2019), 2340-2358.
[3] Ke Chen, Qin Li, Jianfeng Lu and Stephen J. Wright, *Random Sampling and Efficient Algorithms for Multiscale PDEs*, SIAM J. Sci. Comput. **42(5)** (2020), A2974-A3005.
[4] Shi Chen, Qin Li, Jianfeng Lu and Stephen J. Wright, *Manifold learning and Nonlinear homogenization*, arXiv: 2011.00568., **2020**.

An inverse problem for chemotaxis

Kathrin Hellmuth
(joint work with Christian Klingenberg, Qin Li, Min Tang)

Inverse problems describe the question of recovering parts of a model from experimental observations made in nature. In this work, we consider PDEs where a coefficient shall be recovered given the initial data and measurements of the corresponding solution. Since this question is often ill-posed, several regularization techniques were developed. The overall goal of this project is to study the approximation properties of kinetic equations and their macroscopic scaling limits in the inverse setting which might lead to new approaches in regularization.

At first, we investigate this in the framework of mathematical biology describing bacterial movement. The convergence for the forward models for a classical chemotaxis equations to its macroscopic diffusion limit, a Keller-Segel system, was studied by Chalub et al. [1]. We now consider the corresponding Bayesian inverse problems where we are interested in recovering the tumbling kernel describing the velocity jump process in the kinetic equation. This tumbling kernel also determines the drift and diffusion coefficient in the macroscopic equation and thus has its pendent in the macroscopic inverse problem. We were able to show that under some assumptions the posterior distributions arising from both inverse problems converge in a Kullback-Leibler divergence.

1. The Bayesian approach

Within the last years the Bayesian point of view on inverse problems became popular. As explained in Stuart [4], in this approach, the experimental measurements y are modelled to be random variables

$$y = G(c) + n$$

depending on the to be determined random PDE coefficient c by a known deterministic measurement function G and some random noise n of known distribution. The a prior distribution μ_0 is inferred to the coefficient c to incorporate the prior belief. The solution to this problem is then - under some conditions to provide its existence - given by the posterior distribution

$$\mu^y(c) = \frac{1}{Z}\mu^c(y)\mu_0(c)$$

representing the probability of the coefficient taking the value c given the observed data y. The likelihood $\mu^c(y)$ denotes the probability of occurrence of the data y if a model with parameter c is considered and Z is a normalization constant.

2. Forward Chemotaxis and Keller-Segel model

In our research we apply this framework to the subject of chemotaxis. With this term one describes the movement of bacteria cells driven by an attracting chemical substance as described e.g. in Perthame [3]. A classical model is the kinetic chemotaxis equation on the evolution of the density of bacteria $f(x, t, v)$

with velocity $v \in V$ at space point $x \in \mathbb{R}^3$ and time $t \geq 0$. The velocity space V is some spherically symmetric compact subset of $\mathbb{R}^3$. In a parabolic scaling, the equation reads

$$\varepsilon^2 \frac{\partial}{\partial t} f_\varepsilon(x,t,v) + \varepsilon v \cdot \nabla_x f_\varepsilon(x,t,v) = \int_V K_\varepsilon(c_\varepsilon, v, v', x, t) f_\varepsilon(x,t,v') - K_\varepsilon(c_\varepsilon, v', v, x, t) f_\varepsilon(x,t,v) dv'. \tag{1}$$

The right hand side of equation (1) represents the velocity jump by tumbling with tumbling kernel K_ε. It models the way the bacteria change their direction by tumbling before running straight in the new direction again. The tumbling kernel depends on the chemoattractant concentration $c_\varepsilon = c_\varepsilon(x,t)$ which can e.g. be modelled by the parabolic equation

$$-\Delta c_\varepsilon(x,t) = \int_V f_\varepsilon(x,t,v) dv := \rho_\varepsilon(x,t). \tag{2}$$

Deploying the diffusion limit to the coupled system (1), (2), on the macroscopic level a Keller-Segel model describes the density of the bacteria $\rho = \rho(x,t)$

$$\frac{\partial}{\partial t}\rho - \nabla \cdot (D \cdot \nabla \rho) + \nabla \cdot (\rho \chi \cdot \nabla c) = 0. \tag{3}$$

In this model $\chi = \chi(c, \rho)$ is the sensitivity of bacteria with respect to the chemoattractant and $D = D(c, \rho)$ is the diffusion coefficient. They are determined by the zeroth and first order terms in ε of the tumbling kernel K_ε in the chemotaxis equation (1), see e.g. Chalub et al. [1].

In a first step, we consider the model where the chemoattractant is not produced or consumed by the bacteria but a known function, i.e. we just consider the macroscopic or kinetic equation for the bacteria density without coupling of equation (2). Slightly adapting the requirements in [1], one sees that the convergence of these models also holds.

3. The inverse problems for chemotaxis and Keller-Segel

In the inverse problem we would like to determine the tumbling kernel K_ε which gives insight to the bacteria's 'choice' to turn from running to tumbling and selecting a new velocity. Since only the zeroth and first order terms K_0 and K_1 in ε of the tumbling kernel $K_\varepsilon = K_0 + \varepsilon K_1 + O(\varepsilon^2)$ contribute to the Keller-Segel model, we restrict our investigations to tumbling kernels of the form $K_\varepsilon = K_0 + \varepsilon K_1$.

The measurements of the bacteria density are modelled to be of the form

$$y_{mn}(K_0, K_1) = G^{chem}_{mn}(K_0, K_1) + n_{mn} = \int_{\mathbb{R}^3} \int_V f^{(n)}_\varepsilon(x, t_m, v)\, dv \chi_m(x)\, dx + n_{mn},$$

$$\tilde{y}_{mn}(K_0, K_1) = G^{KS}_{mn}(K_0, K_1) + \tilde{n}_{mn} = \int_{\mathbb{R}^3} \rho^{(n)}(x, t_m) \chi_m(x)\, dx + \tilde{n}_{mn}$$

for $m = 1, ..., M, n = 1, ..., N$, $M, N \in \mathbb{N}$, where $f^{(n)}_\varepsilon$ and $\rho^{(n)}$ are the solution to the scaled chemotaxis equation (1) with initial data $f^{(n)}_0(x,v) \in L^1 \cap L^\infty(\mathbb{R}^3 \times V)$

and the macroscopic equation (3) with initial data $\rho_0^{(n)} = \int_V f_0^{(n)}\, dv$ respectively. The measurements are thus derived at a precise point in time $t_m \in (0,T)$ and a test function $\chi_m \in C_c$ in space. The measurement errors n_{mn} and $\tilde{n}_{mn}$ are assumed to be iid Gaussian with mean 0 and variance γ^2. The measurements depend on K_0, K_1 through the evolution of f_ε and ρ.

In the Bayesian setting, we assume that an a prior distribution μ_0 of the tumbling kernel components (K_0, K_1) is given. Then the posterior distributions are

$$\begin{aligned}\mu^y_{chem}(K_0,K_1) &= \frac{1}{Z_{chem}} \exp\left(-\frac{1}{2\gamma^2}\|y - G^{chem}(K_0,K_1)\|^2\right)\mu_0(K_0,K_1) \quad \text{and}\\ \mu^y_{KS}(K_0,K_1) &= \frac{1}{Z_{KS}} \exp\left(-\frac{1}{2\gamma^2}\|y - G^{KS}(K_0,K_1)\|^2\right)\mu_0(K_0,K_1).\end{aligned}$$

4. Inverse limit behaviour

Since the Keller Segel model is the macroscopic limit of the scaled chemotaxis equation, we investigate the inverse problems for their limiting behaviour when considering the same measurement data y. This is done in analogy to a paper of Newton et al. [2]. This addresses the question if the inverse models also approximate each other.

To ensure the existence of solutions to the chemotaxis and the Keller-Segel like equation and the requirements for forward model convergence, we assume

- K_0, K_1 to be continuously differentiable and bounded,
- K_0 to be symmetric in v, v' and bounded away from zero and
- K_1 to be antisymmetric in v, v'

The admissible set $\mathcal{A}$ collects all such pairs (K_0, K_1). By these assumptions, the posterior distributions are absolutely continuous w.r.t. each other and depend continuously on the data y. For the chemotaxis model, we showed the well-definedness and thus well-posedness of the posterior solution whereas the well-definedness for the Keller-Segel posterior is work in progress.

We consider the distance of the posterior measures in the Kullback-Leibler divergence

$$d_{KL}(\mu^y_{chem}, \mu^y_{KS}) = \int_{\mathcal{A}} \left(\log \frac{d\mu^y_{chem}}{d\mu^y_{KS}}(K_0,K_1)\right) d\mu^y_{KS}(K_0,K_1).$$

Under the above assumptions, we could show convergence of the posterior measures in this distances confirming the connection between the models also in the inverse setting and enabling approximations for small ε.

References

[1] F. Chalub, P. Markowich, B. Perthame and C. Schmeiser *Kinetic Models for Chemotaxis and their Drift-Diffusion Limits*, Monatsh. Math. **142** (2004), 123–141.
[2] K. Chen, Q. Li and L. Wang, *Diffusive optical tomography in the Bayesian framework*, Multiscale Modeling & Simulation **18** no.2 (2020), 589–611.
[3] B. Perthame, *Transport equations in biology*, Springer Science & Business Media (2006).
[4] A. M. Stuart, *Inverse problems: A Bayesian perspective*, Acta Numerica **19** (2010), 451–559.

Reporter: Lena Baumann

Participants

Dr. Gi-Chan Bae
Department of Mathematical Sciences
Seoul National University
Seoul 151-747
KOREA, REPUBLIC OF

Dr. Wasilij Barsukow
Max-Planck-Institut für Plasmaphysik (IPP)
NMPP
Boltzmannstraße 2
85748 Garching bei München
GERMANY

Lena Baumann
Institut für Mathematik
Universität Würzburg
Emil-Fischer-Strasse 40
97074 Würzburg
GERMANY

Claudius Birke
Institut für Mathematik
Universität Würzburg
Emil-Fischer-Strasse 40
97074 Würzburg
GERMANY

Dr. Philipp Edelmann
Los Alamos National Laboratory
Computer Research Dept.
Mail Stop B 265
Los Alamos, NM 87545
UNITED STATES

Prof. Dr. Eduard Feireisl
Institute of Mathematics of the AS CR
Charles University
Žitná 25
115 67 Praha 1
CZECH REPUBLIC

Dr. Cory Hauck
Oak Ridge National Laboratory
Oak Ridge, TN 37831
UNITED STATES

Kathrin Hellmuth
Institut für Mathematik
Universität Würzburg
Emil-Fischer-Strasse 40
97074 Würzburg
GERMANY

Eva Horlebein
Institut für Mathematik
Universität Würzburg
Emil-Fischer-Strasse 40
97074 Würzburg
GERMANY

Farah Kanbar
Institut für Mathematik
Universität Würzburg
Emil-Fischer-Str. 40
97074 Würzburg
GERMANY

Prof. Dr. Christian Klingenberg
Institut für Mathematik
Universität Würzburg
Emil-Fischer-Strasse 40
97074 Würzburg
GERMANY

Prof. Dr. Ru-Yu Lai
School of Mathematics
University of Minnesota
127 Vincent Hall
206 Church Street S. E.
Minneapolis, MN 55455
UNITED STATES

Dr. Qin Li
Department of Mathematics
University of Wisconsin-Madison
480 Lincoln Drive
Madison, WI 53706-1388
UNITED STATES

Simon Markfelder
Centre for Mathematical Sciences
University of Cambridge
Wilberforce Road
Cambridge CB3 0WB
UNITED KINGDOM

Dr. Marlies Pirner
Institut für Mathematik
Universität Würzburg
Emil-Fischer-Str. 40
97074 Würzburg
GERMANY

Prof. Dr. Min Tang
Institute of Natural Sciences
Shanghai Jiaotong University
No. 800 Dongchuan Road, Minhang District
Shanghai Shi 200 240
CHINA

Sandra Warnecke
Institut für Mathematik
Universität Würzburg
Emil-Fischer-Str. 40
97074 Würzburg
GERMANY

Prof. Dr. Seok-Bae Yun
Department of Mathematics
Sungkyunkwan University
Suwon 440-146
KOREA, REPUBLIC OF